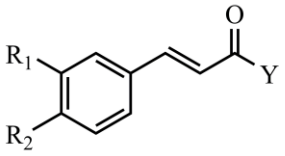
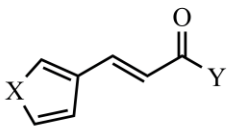
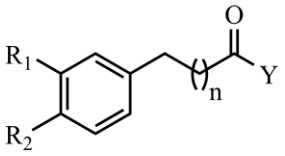
Table 1. Biological activity of tested compounds.



1-6, 9-12



7-8



17, 21-28, 30-31, 34, 36

Compound	R_1	R_2	n	Y	X	PqsD IC_{50} (µM)	% HHQ inhibition in PA14 *pqsH*⁻ at 250µM	cLogP[a]
1	H	H		OH		33% @50µM	n.i.	2.13
2	H	OH		OH		30% @50µM	n.i.	1.63
3	OH	H		OH		n.i.	n.d.	1.63
4	OH	OH		OH		26% @50µM	10% @500µM	1.32
5	OMe	OH		OH		n.i.	n.d.	1.70
6	F	F		OH		18% @50µM	n.d.	2.25
7				OH	S	12% @50µM	n.i.	1.03
8				OH	O	12% @50µM	n.d.	1.33
9	H	H		OMe		n.i.	n.d.	2.49
10	H	OH		OMe		22% @50µM	n.i.	1.74
11	OH	OH		OMe		51 ± 4	31 ± 2	2.01
12	F	F		OMe		n.i.	n.i.	2.67
17	OH	OH	1	OH		27 ± 2	n.i.	1.01
21	H	OH	1	OMe		n.i.	n.d.	1.89
22	H	Me	1	OMe		n.i.	n.d.	2.71
23	H	NO_2	1	OMe		n.i.	n.d.	2.24
24	H	NH_2	1	OMe		n.i.	n.d.	1.64
25	OH	OH	1	OMe		23 ± 1	17 ± 1	2.00
26	OH	OH	1	OEt		14 ± 1	17 ± 1	2.47
27	OH	OH	1	OiPr		8.6 ± 0.6	16	2.77
28	OH	OH	0	OMe		23 ± 1	24 ± 3	1.31
30	OH	OH	2	OMe		7.9 ± 0.2	18 ± 2	2.47
31	O–CH_2–O		1	OMe		37% @50µM	n.i.	2.33
34	OH	OH	1	NHMe		20 ± 4	n.i.	0.76
36	OH	OH	1	OCH_2Ph		5.9 ± 1.2	n.i.	3.13

n.d. = not determined.

n.i. = no significant inhibition (<10%).

[a] Calculated by ACD/Labs 2012 using ACD/LogP GALAS algorithm.